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Analyticity for some operator functions from statistical quantum mechanics

Dedicated to Günter Albinus

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Abstract

For rather general thermodynamic equilibrium distribution functions the density of a statistical ensemble of quantum mechanical particles depends analytically on the potential in the Schödinger operator describing the quantum system. A key to the proof is that the resolvent to a power less than one of an elliptic operator with non-smooth coefficients, and mixed Dirichlet/Neumann boundary conditions on a bounded up to three-dimensional Lipschitz domain factorizes over the space of essentially bounded functions.

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1 Introduction

In the investigation of many-particle systems, in particular electronic ones, the Kohn-Sham equations of Density Functional Theory are a common tool, cf. e. g. [29], [1], [38], [10], [12], [28]. The particle density $\mathcal{N}$ in a statistical ensemble of (identical) quantum mechanical systems is given by

$$\mathcal{N}(V)(x) = \sum_{k=1}^{\infty} f(\lambda_k)|\psi_k(x)|^2, \tag{1.1}$$

where H_0 is the kinetic part of a Schrödinger operator, and V a variable real potential; ψ_k and λ_k are the eigenfunctions and eigenvalues of the Schrödinger operator $H_0 + V$. The argument x in (1.1) is a point in real space, and f is a thermodynamic equilibrium distribution function, for instance the Fermi function $f(s) = 1/(1+e^s)$. If H_0, V, and f are such that the operator $f(H_0+V)$ is nuclear, then the particle density $\mathcal{N}(V)$ can be represented in terms of $f(H_0+V)$ by $\int_\Omega \mathcal{N}(V)W\,dx = \operatorname{tr}\big(Wf(H_0+V)\big)$ for all $W \in L^\infty$, cf. e. g. [22]. The analysis of the Kohn-Sham system is based on properties such as monotonicity, and differentiability of the operator function $f(H_0+V)$ in its dependence on the Schrödinger potential V, cf. e. g. [34], [36], [24], [25], [26]. In [22] we have demonstrated that the functional

$$\phi(V) \stackrel{\text{def}}{=} \operatorname{tr}\big(F(H_0+V)\big), \quad \text{where } F(t) \stackrel{\text{def}}{=} \int_t^\infty f(s)\,ds,$$

is convex and Fréchet differentiable. The functional ϕ represents the free energy of a statistical ensemble of quantum mechanical systems, and the gradient of this functional is the statistical operator (density matrix) $\partial\phi(V) = f(H_0+V)$, cf. [22]. For special cases the convexity and differentiability of the functional ϕ has been proved already in 1990 independently by Caussinac et al. [6] and Nier [34]. These results have been generalized, i. e. in [36], [35], [23], [24], [25], [26]. Furthermore, Nier has shown, cf. [36], [35], that the particle density operator $\mathcal{N}$ is infinitely often Fréchet differentiable as a mapping from $W^{1,2}$ into $W^{-1,2}$.

Here we are interested in the *analyticity* of $\mathcal{N}$ for a wider class of Schrödinger operators and for function spaces allowing for more general Schrödinger potentials. Moreover, we pass to realisations of the underlying Hilbert space in the quantum mechanics by function spaces adapted to real world problems. More precisely, we regard function spaces with respect to spatial domains which are just bounded Lipschitz domains. This requires inter alia to prove in such a non-smooth situation that the resolvent of an elliptic operator to a power less than 1 maps L^2 continously into L^∞, cf. Theorem 4.3 — a new result which is of interest independently of our usage here.

The proper choice of boundary conditions for the eigenfunctions of the Schrödinger operator in quantum mechanical calculations on a bounded domain of real space is still in debate, cf. e. g. [42] and [43]. Since homogeneous Dirichlet and Neumann boundary conditions may be of interest, we allow for both of them. Moreover, we also want to include the quasi two dimensional case of a cylindrical symmetric domain. That's why we regard mixed Dirichlet/Neumann boundary conditions.

The analyticity of the particle density operator $\mathcal{N}$, which is equivalent to the analyticity of the operator function $V \mapsto f(H_0+V)$, comes to bear in establishing steadily converging iteration schemes for the Kohn-Sham system. Indeed, analyticity enables to prove a generalized Łojasiewicz–Simon inequality, cf. [8], [14], [16]. This has been used by Gajewski and Griepentrog in the set-up of a descent method for the free energy of multicomponent systems [16].

2 Preliminaries

Throughout this paper we regard the real space representation of the quantum mechanics governing the particle system on a bounded up to three dimensional spatial domain Ω, i. e. we deal with a Schrödinger operator on the Hilbert space $L^2(\Omega)$. In order to simplify notations, we omit the indication for Ω in the symbol for a function space referring to Ω. Moreover, we write $L^2_{\mathbb{R}}$ for the real part of $L^2 = L^2(\Omega)$. Finally, c denotes a generic, positive constant, not always of the same value.

We always make the following two general assumptions for the spatial domain Ω and the coefficient function μ of the Schrödinger operator $H_0 = -\nabla\cdot(\mu\nabla)$. In the context of semiconductor physics H_0 is an effective mass Hamiltonian in Ben–Daniel–Duke form [2], and μ is the inverse effective mass, cf. [40, Ch. 1].

Assumption 2.1. Ω is an interval or a bounded Lipschitz domain in $\mathbb{R}^d$, cf. e. g. [33, Ch. 1.1.9] or [18, Defn. 1.2.1.2]. We regard one–, two–, and three-dimensional spatial domains: i. e. $d \in \{1, 2, 3\}$, cf. Remark 4.4. — Π is an arbitrary closed subset of the boundary $\partial\Omega$.

Assumption 2.2. The coefficient function μ on Ω is Lebesgue measurable, bounded, elliptic and takes its values in the set of real, symmetric $d \times d$ matrices.

Definition 2.3. $W^{1,2}_\Pi$ denotes the $W^{1,2}(\Omega)$–closure of the set

$$\left\{\psi|_\Omega : \psi \in C^\infty(\mathbb{R}^d),\, \operatorname{supp}\psi \cap \Pi = \emptyset\right\}.$$

H_0 is the selfadjoint operator on $L^2(\Omega)$ which corresponds to the quadratic form

$$W^{1,2}_\Pi \ni \psi \mapsto \int_\Omega \mu\nabla\psi \cdot \nabla\bar{\psi}\, dx.$$

We denote the domain of H_0 by $\mathcal{D}$.

Remark 2.4. The boundary conditions associated with H_0 are a homogeneous Dirichlet condition on Π and a Neumann condition — in the sense of distributions — on $\partial\Omega \setminus \Pi$. As, in particular, Π may be the empty set, Assumption 2.1 allows for a Neumann condition on all the boundary of the spatial domain Ω.

For two Banach spaces we denote the space of linear, continuous operators from X into Y by $\mathcal{B}(X;Y)$. If $X = Y$, we abbreviate $\mathcal{B}(X;X) = \mathcal{B}(X)$, and if $X = L^2$, we once more abbreviate $\mathcal{B}(L^2) = \mathcal{B}$. The ideal of compact operators within $\mathcal{B}$ is denoted by $\mathcal{B}_\infty$, and $\mathcal{B}_r$, $r \in [1, \infty[$, stands for the Schatten class with index r in $\mathcal{B}_\infty$.

In the sequel we always identify a function from L^2 with the multiplication operator induced by this function. In this sense L^∞ is embedded into $\mathcal{B}$.

Definition 2.5. Following Vaĭnberg [44, Ch. 22], cf. also [7], [20, Ch. III.3], we call a mapping $F_j : X \to Y$, $j \in \mathbb{N}$, between two Banach spaces a *j-power mapping*, if there is a continuous, mapping $G_j : X \oplus \ldots \oplus X \to Y$ which is linear in each of its j arguments, such that $F_j(\mathfrak{x}) = G_j(\mathfrak{x}, \ldots, \mathfrak{x})$. A mapping $F : X \to Y$ is called *analytic* in a point $\mathfrak{x}_0 \in X$ if there is a ball $B \subset X$ around zero and a sequence $\{F_j\}_{j\in\mathbb{N}}$ of j-power mappings such that

$$F(\mathfrak{x}_0 + \mathfrak{x}) = F(\mathfrak{x}_0) + \sum_{j=1}^{\infty} F_j(\mathfrak{x}) \quad \text{for all } \mathfrak{x} \in B,$$

and the series converges in Y uniformly for $\mathfrak{x} \in B$.

Analytic mappings possess many properties, analogous to those of classical holomorphic functions, cf. [44, Ch. 22] for details.

3 Main result

First we rigorously define the particle density (1.1) in a statistical ensemble of quantum mechanical systems in thermodynamic equilibrium, cf. e. g. [1] [10], [28], [22] and the references cited there.

Definition 3.1. Let H_0 be the operator from Definition 2.3, and let V be a real potential such that the operator $H_0 + V$ is semibounded from below, selfadjoint and has pure point spectrum. If $f : \mathbb{R} \to \mathbb{R}_+$ is a sufficiently decaying distribution function so that $f(H_0 + V) \in \mathcal{B}_1$, then we define the corresponding particle density $\mathcal{N}(V)$ by

$$\int_\Omega \mathcal{N}(V) W \, dx = \operatorname{tr}\big(W f(H_0 + V)\big) \quad \text{for all } W \in L^\infty. \tag{3.1}$$

Remark 3.2. According to [22, Thm. 36] $\mathcal{N}(V)$ is a function in the non-negative cone of $L^1_{\mathbb{R}}$. If $\{\lambda_k\}$ is the sequence of eigenvalues for $H_0 + V$ (counting multiplicity) and $\{\psi_k\}$ is the corresponding sequence of (normalized) eigenvectors, then $\mathcal{N}(V)$ equivalently can be expressed by (1.1).

Definition 3.3. For every $\alpha > 0$ we denote by Υ_α the contour

$$\{\lambda : \lambda = s \pm i\alpha s, \, s \geq 0\}$$

with positive orientation. $\mathcal{P}_\alpha$ stands for the set of points in $\mathbb{C}$ which are enclosed by Υ_α, i. e.

$$\mathcal{P}_\alpha \stackrel{\text{def}}{=} \{\lambda_1 + i\lambda_2 : \lambda_1 > 0, \, |\lambda_2| < \alpha\lambda_1 \}.$$

The thermodynamic equilibrium distribution function f of the complex quantum system represents the underlying statistics, cf. e. g. [40, Ch. 1.12] or [21, Ch. 6.3]. Generally, for an electron gas in the three dimensional space, f is the Fermi function

$$f(s) = 1/(1 + e^s).$$

For a two– or one-dimensional electron gas (i.e. $d = 1$ or $d = 2$) the distribution function is $f(s) = c\,\mathcal{F}_{-1/2}(-s)$ or $f(s) = c\,\mathcal{F}_0(-s)$, respectively, where $\mathcal{F}_r$ is the Fermi–integral

$$\mathcal{F}_r(s) = \tfrac{1}{\Gamma(r+1)} \int_0^\infty \tfrac{t^r}{1+exp(t-s)}\,dt,$$

cf. e. g. [30]. These distribution functions have singularities in the closed left half plane. Thus, one cannot ask f to be holomorphic on the whole complex plane. But, we make the following assumption about the thermodynamic equilibrium distribution function f, which is fulfilled for the above examples.

Assumption 3.4. For every $t \in \mathbb{R}$ there is an $\alpha > 0$ so that the distribution function f is defined and holomorphic on $\mathcal{P}_\alpha - t$. Moreover, there is an $\alpha > 0$ such that

$$\sup_{\lambda \in \mathcal{P}_\alpha} |\lambda^9 f(\lambda)| < \infty.$$

The restriction of f to $\mathbb{R}$ is real-valued and non-negative.

Remark 3.5. From Assumption 3.4 follows in particular that for every $t \in \mathbb{R}$ there is an $\alpha > 0$ such that

$$\sup_{\lambda \in \mathcal{P}_\alpha - t} |\lambda^9 f(\lambda)| < \infty, \quad \text{and} \quad \int_\Upsilon |\lambda|^7 |f(\lambda)|\, d|\lambda|,$$

where Υ is the contour corresponding to $\mathcal{P}_\alpha - t$ in the sense of Definition 3.3. This comes to bear in the proof of Lemma 4.1, cf. Remark 5.7.

Remark 3.6. A distribution function f conforming to Assumption 3.4 satisfies $f(\bar{\lambda}) = \overline{f(\lambda)}$ for all λ from that connected component of the holomorphy domain which contains $\mathbb{R}$.

We now state our main result.

Theorem 3.7. *Let us make the Assumptions 2.1, 2.2 and 3.4. Then the mapping $L^2_{\mathbb{R}} \ni V \mapsto \mathcal{N}(V) \in L^2_{\mathbb{R}}$, cf. Definition 3.1, is analytic in every point $V \in L^2_{\mathbb{R}}$, cf. Definition 2.5.*

4 Auxiliary results

Lemma 4.1. *If A is a selfadjoint operator on a Hilbert space $\mathfrak{H}$ the spectrum of which is contained in $[1,\infty[$, then*

$$\sup_{\lambda\in\Upsilon} \|A(A-\lambda)^{-1}\|_{\mathcal{B}(\mathfrak{H})} \leq \frac{1}{\operatorname{dist}(1,\Upsilon)} \tag{4.1}$$

for all $\Upsilon = \Upsilon_\alpha$ with $\alpha > 0$, cf. Definition 3.3.

Proof. By a classical result, cf. e. g. [27, Ch. V.3.5], one has

$$\|A(A-\lambda)^{-1}\|_{\mathcal{B}(\mathfrak{H})} = \sup_{s\in\operatorname{spec}(A)} \frac{|s|}{|s-\lambda|} \leq \sup_{s\in[1,\infty[} \frac{s}{|s-\lambda|}$$

at least for all $\lambda \in \Upsilon$. This gives

$$\begin{aligned}\sup_{\lambda\in\Upsilon} \|A(A-\lambda)^{-1}\|_{\mathcal{B}(\mathfrak{H})} &\leq \sup_{\lambda\in\Upsilon}\sup_{s\in[1,\infty[} \frac{s}{|s-\lambda|} = \sup_{(\lambda,s)\in\Upsilon\times[1,\infty[} \frac{1}{|1-\frac{\lambda}{s}|} \\ &= \sup_{\lambda\in\Upsilon} \frac{1}{|1-\lambda|} = \frac{1}{\inf_{\lambda\in\Upsilon}|1-\lambda|} = \frac{1}{\operatorname{dist}(1,\Upsilon)}.\end{aligned}$$

□

Proposition 4.2. *(Cf. [37, Thm. 6.10], and [19].) For the operator H_0 from Definition 2.3 the semigroup operators e^{-tH_0}, $t \geq 0$ are integral operators whose kernels $K_t : \Omega\times\Omega \to \mathbb{R}$ allow the Gaussian estimates*

$$0 \leq K_t(x,y) \leq \gamma\, t^{-\frac{d}{2}} e^{\varepsilon t} e^{-b\frac{|x-y|^2}{t}} \quad \textit{for almost all } (x,y)\in\Omega\times\Omega, \tag{4.2}$$

where γ, b, and ε are non-negative constants related to H_0.

Theorem 4.3. *Let again H_0 be the operator from Definition 2.3. For every $\theta \in]\frac{d}{4},1]$, the operator $(H_0+1)^{-\theta}$ maps L^2 continuously into L^∞.*

Proof. As e^{-tH_0} admits the Gaussian estimate (4.2), the kernels $L_t : \Omega\times\Omega \to \mathbb{R}$ belonging to the semigroup operators $e^{-t(H_0+\delta)}$ satisfy the estimate

$$0 \leq L_t(x,y) \leq \gamma\, t^{-\frac{d}{2}} e^{-t(\delta-\varepsilon)} e^{-b\frac{|x-y|^2}{t}} \tag{4.3}$$

for almost all $(x,y)\in\Omega\times\Omega$, and for all $t \geq 0$ and $\delta \geq 0$. By means of the representation formula

$$(H_0+\delta)^{-\theta} = \frac{1}{\Gamma(\theta)} \int_0^\infty t^{\theta-1} e^{-t(H_0+\delta)}\,dt,$$

cf. [39, Ch. 2.6], one estimates for any $\psi \in L^2$

$$\|(H_0+\delta)^{-\theta}\psi\|_{L^\infty} \le \frac{1}{\Gamma(\theta)} \Big\| \int_0^\infty t^{\theta-1} e^{-t(H_0+\delta)}\psi\, dt \Big\|_{L^\infty}$$
$$\le \frac{1}{\Gamma(\theta)} \int_0^\infty t^{\theta-1} \big\| e^{-t(H_0+\delta)}\psi \big\|_{L^\infty}\, dt. \quad (4.4)$$

Using now the Gaussian estimate (4.3), one finds

$$\begin{aligned}\|e^{-t(H_0+\delta)}\psi\|_{L^\infty} &= \operatorname*{vrai\,sup}_{y\in\Omega} \big| \textstyle\int_\Omega L_t(y,x)\,\psi(x)\,dx \big| \\ &\le \operatorname*{vrai\,sup}_{y\in\Omega} \sqrt{\textstyle\int_\Omega |L_t(y,x)|^2\,dx}\ \|\psi\|_{L^2} \\ &\le \gamma\, t^{-\frac{d}{2}}\, e^{-t(\delta-\varepsilon)}\, \|\psi\|_{L^2} \operatorname*{vrai\,sup}_{y\in\Omega} \sqrt{\textstyle\int_\Omega e^{-2b\frac{|x-y|^2}{t}}\, dx} \\ &\le \gamma\, t^{-\frac{d}{2}}\, e^{-t(\delta-\varepsilon)}\, \|\psi\|_{L^2} \operatorname*{vrai\,sup}_{y\in\Omega} \sqrt{\textstyle\int_{\mathbb{R}^d} e^{-2b\frac{|x-y|^2}{t}}\, dx} \\ &= \gamma \left(\frac{\pi}{2b}\right)^{d/4} e^{-t(\delta-\varepsilon)} t^{-d/4} \|\psi\|_{L^2}.\end{aligned}$$

Nota bene $\int_{\mathbb{R}^d} e^{-2b\,|x-y|^2/t}\,dx = \left(\frac{t\pi}{2b}\right)^{d/2}$, cf. the multivariate Gaussian distribution. Thus, (4.4) can be continued

$$\|(H_0+\delta)^{-\theta}\psi\|_{L^\infty} \le \frac{\gamma}{\Gamma(\theta)} \left(\frac{\pi}{2b}\right)^{d/4} \int_0^\infty t^{\theta-1-d/4} e^{-t(\delta-\varepsilon)}\, dt\ \|\psi\|_{L^2}. \quad (4.5)$$

The right hand side of (4.5) is finite if $\delta > \varepsilon$ and $\theta > d/4$. Thus, in this case $(H_0+\delta)^{-\theta} \in \mathcal{B}(L^2; L^\infty)$. Finally, one obtains

$$\|(H_0+1)^{-\theta}\|_{\mathcal{B}(L^2;L^\infty)} \le \|(H_0+\delta)^{-\theta}\|_{\mathcal{B}(L^2;L^\infty)} \|(H_0+\delta)^{\theta}(H_0+1)^{-\theta}\|_{\mathcal{B}},$$

where the second factor is finite due to the positivity of H_0 and functional calculus. □

Remark 4.4. Theorem 4.3 restricts the dimension of the spatial domain Ω to 1, 2, and 3, cf. also [36]. Indeed, for $d \ge 4$ the operators $(H_0+1)^{-1}$ generically do not allow a factorization over L^∞. By a classical result, cf. [31, Ch. I.2] $(H_0+1)^{-1} \in \mathcal{B}(L^p; L^\infty)$ in general requires $p > \frac{d}{2}$. Yet, the factorization of $(H_0+1)^{-\theta}$ over L^∞ even for some $\theta < 1$ is crucial in the following considerations.

Theorem 4.5. *For the operator H_0 from Definition 2.3 the resolvent is in a Schatten class, more precisely: $(H_0+1)^{-1} \in \mathcal{B}_r$ for every $r > d/2$.*

Proof. For every $\theta \in]\frac{d}{4}, 1]$, the operator $(H_0 + 1)^{-\theta} : L^2 \to L^2$ admits a factorization over L^∞, cf. Theorem 4.3. Hence, it must be Hilbert-Schmidt by a classical factorization theorem, cf. [32, Prop. 6.3] or [11, Cor. 4.11], which implies the assertion. □

Remark 4.6. The argument in the proof of Theorem 4.5 additionally shows that the left end $\theta = d/4$ of the θ–interval in Theorem 4.3 cannot be improved. Otherwise, one could conclude $(H_0 + 1)^{-d/4} \in \mathcal{B}_2$, or, equivalently, $(H_0 + 1)^{-d/2} \in \mathcal{B}_1$. However, this is wrong in general, according to Weyl's asymptotic law for eigenvalues of the Laplacian.

Remark 4.7. For a Schrödinger operator H_0 with a homogeneous Dirichlet boundary condition the assertion of Theorem 4.5 has been proved by BIRMAN and SOLOMYAK even for an arbitrary domain Ω, cf. [4, Ch. 11.3] and [3]. The case of a Neumann boundary condition has been treated in [3], [4], [5], provided that the underlying domain Ω is a $W^{1,2}$ extension domain, i. e. if there is a linear, continuous extension operator from $W^{1,2}(\Omega)$ to $W^{1,2}(\mathbb{R}^d)$. Indeed, this result holds true also for Lipschitz domains, cf. [17, Thm. 3.10], and [33, Ch. 1.1.16]. Having the Dirichlet and Neumann case at hand, one easily carries this over to the case of mixed boundary conditions by the classical comparison principle, cf. [9, Ch. 6.2]. It is interesting to note that the proof of the Gaussian estimates in Proposition 4.2 also fundamentally rests on the same extension property for the underlying domain Ω.

Corollary 4.8. *For the operator H_0 from Definition 2.3, and for every $V \in L^2$ the operator $V(H_0 + 1)^{-1} : L^2 \to L^2$ is not only bounded, but compact and belongs to the Schatten class $\mathcal{B}_7$. More precisely, one can estimate*

$$\begin{aligned} \|V(H_0 + 1)^{-1}\|_{\mathcal{B}} &\le \|V(H_0 + 1)^{-1}\|_{\mathcal{B}_7} \\ &\le \|V\|_{L^2} \|(H_0 + 1)^{-10/13}\|_{\mathcal{B}(L^2;L^\infty)} \|(H_0 + 1)^{-3/13}\|_{\mathcal{B}_7} < \infty. \end{aligned} \tag{4.6}$$

Proof. $\|(H_0 + 1)^{-10/13}\|_{\mathcal{B}(L^2;L^\infty)}$ is finite since $10/13 > 3/4 \ge d/4$, cf. Theorem 4.3. Further, according to Theorem 4.5, $(H_0 + 1)^{-1}$ belongs to the Schatten class $\mathcal{B}_r$ for every $r > 3/2 \ge d/2$, in particular $(H_0 + 1)^{-1} \in \mathcal{B}_{21/13}$. Hence, $(H_0 + 1)^{-3/13}$ is in the Schatten class $\mathcal{B}_7$. □

Lemma 4.9. *For the operator H_0 from Definition 2.3, and for every $V \in L^2$ the multiplication operator induced by V is infinitesimally small with respect to $H_0 + 1$.*

Proof. Due to Theorem 4.3 one can estimate

$$\|V\psi\|_{L^2} \le \|V\|_{L^2} \|\psi\|_{L^\infty} \le c\|V\|_{L^2} \|(H_0 + 1)^{4/5}\psi\|_{L^2}$$

for all $\psi \in \mathcal{D} = \operatorname{dom} H_0$. Since $H_0 + 1$ is selfadjoint and positive, the right hand side may be further estimated by

$$c\,\|V\|_{L^2}\,\|\psi\|_{L^2}^{1/5}\,\|(H_0+1)\psi\|_{L^2}^{4/5},$$

cf. [39, Ch. 2.6 Th. 6.10]. According to Young's inequality, this is not larger than

$$\epsilon\|(H_0+1)\psi\|_{L^2} + \left(\tfrac{1}{\epsilon}\right)^4 (c\|V\|_{L^2})^5 \|\psi\|_{L^2}$$

for any $\epsilon > 0$. □

Corollary 4.10. *For every potential $V \in L^2_{\mathbb{R}}$ the operator $H_0 + V$*

- *is selfadjoint like H_0,*
- *has $\mathcal{D} = \operatorname{dom} H_0$ as its domain,*
- *has, like H_0, a pure point spectrum,*
- *is semibounded from below, and the corresponding lower form bounds may be taken uniformly with respect to bounded sets in $L^2_{\mathbb{R}}$.*

Proof. The first three items follow from Lemma 4.9 by classical perturbation theorems. The last assertion has been proved in [25, Prop. 3.3] for $d = 1$, and in [26, Prop. 3.4] for $d = 2$ and $d = 3$. □

Corollary 4.11. *If $V \in L^2_{\mathbb{R}}$ and $\tau \in \mathbb{R} \setminus \operatorname{spec}(H_0 + V)$, then*

$$\|(H_0+1)(H_0+V-\tau)^{-1}\|_{\mathcal{B}} < \infty. \tag{4.7}$$

If additionally $W \in L^2_{\mathbb{R}}$, then

$$\begin{aligned}&\|W(H_0+V-\tau)^{-1}\|_{\mathcal{B}}\\ &\qquad \le \|W\|_{L^2}\|(H_0+1)^{-1}\|_{\mathcal{B}(L^2;L^\infty)}\|(H_0+1)(H_0+V-\tau)^{-1}\|_{\mathcal{B}} < \infty\end{aligned} \tag{4.8}$$

and

$$\begin{aligned}\|W(H_0+V-\tau)^{-1}\|_{\mathcal{B}_7} \le \|W\|_{L^2}\|(H_0+1)^{-\frac{10}{13}}\|_{\mathcal{B}(L^2;L^\infty)}\|(H_0+1)^{-\frac{3}{13}}\|_{\mathcal{B}_7}\times&\\ \times\|(H_0+1)(H_0+V-\tau)^{-1}\|_{\mathcal{B}} < \infty.&\end{aligned} \tag{4.9}$$

Proof. $(H_0+V-\tau)(H_0+1)^{-1} : L^2 \to L^2$ is continuous and bijective. Hence, by the Open Mapping Theorem, its inverse must be continuous, which proves (4.7). Now, (4.8) and (4.9) follow from Theorem 4.3, Theorem 4.5, and Corollary 4.8, respectively, by means of (4.7). □

Lemma 4.12. *We regard the operator H_0 from Definition 2.3. Suppose V_1, $V_2 \in L^2_{\mathbb{R}}$. Moreover, let us assume that $f : \mathbb{R} \to \mathbb{R}$ is bounded on bounded sets and satisfies $\sup_{t\in[0,\infty[} t^3|f(t)| < \infty$. Then $(H_0 + V_1)f(H_0 + V_2) \in \mathcal{B}_1$.*

Proof. For $\tau \in \mathbb{R} \setminus \operatorname{spec}(H_0 + V_2)$ one estimates:

$$\begin{aligned}
&\|(H_0 + V_1)f(H_0 + V_2)\|_{\mathcal{B}_1}\\
&\le \|(H_0 + V_2 - \tau)f(H_0 + V_2)\|_{\mathcal{B}_1} + \|(V_1 - V_2 + \tau)f(H_0 + V_2)\|_{\mathcal{B}_1}\\
&\le \big(1 + \|(V_1 - V_2 + \tau)(H_0 + V_2 - \tau)^{-1}\|_{\mathcal{B}}\big)\times\\
&\qquad\qquad \times \|(H_0 + V_2 - \tau)^{-1}\|^2_{\mathcal{B}_2}\|(H_0 + V_2 - \tau)^3 f(H_0 + V_2)\|_{\mathcal{B}}
\end{aligned}$$

According to Corollary 4.11 the term $\|(V_1 - V_2 + \tau)(H_0 + V_2 - \tau)^{-1}\|_{\mathcal{B}}$ is bounded. Further one can estimate

$$\|(H_0 + V_2 - \tau)^{-1}\|_{\mathcal{B}_2} \le \|(H_0 + 1)^{-1}\|_{\mathcal{B}_2}\|(H_0 + 1)(H_0 + V_2 - \tau)^{-1}\|_{\mathcal{B}} < \infty.$$

Finally,

$$\|(H_0 + V_2 - \tau)^3 f(H_0 + V_2)\|_{\mathcal{B}} \le \sup_{t\in\operatorname{spec}(H_0+V_2)} (t - \tau)^3|f(t)|$$

is finite due to the precondition on f and the semiboundedness of $H_0 + V_2$ from below. □

Corollary 4.13. *If f is a distribution function which meets the preconditions from Lemma 4.12, and $V \in L^2_{\mathbb{R}}$, then $\mathcal{N}(V) \in L^2_{\mathbb{R}}$, where $\mathcal{N}(V)$ is according to Definition 3.1. Thus,* (3.1) *extends to all functions $W \in L^2$:*

$$\int_\Omega \mathcal{N}(V)W\,dx = \operatorname{tr}\big(Wf(H_0 + V)\big) \quad \textit{for all } W \in L^2. \tag{4.10}$$

Proof. According to (3.1) there is

$$\begin{aligned}
\|\mathcal{N}(V)\|_{L^2} &= \sup_{W\in L^\infty,\|W\|_{L^2}\le 1} \left|\textstyle\int_\Omega W\mathcal{N}(V)\,dx\right|\\
&= \sup_{W\in L^\infty,\|W\|_{L^2}\le 1} \left|\operatorname{tr}\big(Wf(H_0 + V)\big)\right|\\
&\le \|(H_0 + 1)^{-1}\|_{\mathcal{B}(L^2;L^\infty)}\|(H_0 + 1)f(H_0 + V)\|_{\mathcal{B}_1}.
\end{aligned}$$

This is finite, due to Theorem 4.3 and Lemma 4.12. □

Remark 4.14. Assumption 3.4 entails the precondition of Lemma 4.12 and Corollary 4.13 for the thermodynamic equilibrium distribution function f.

5 Proof of Theorem 3.7

Let us first recall that $\mathcal{B}_1$ is topologically the dual space to $\mathcal{B}_\infty$, and the duality $\mathcal{B}_\infty \times \mathcal{B}_1 \ni (A, C) \mapsto \langle A, C\rangle_{(\mathcal{B}_\infty,\mathcal{B}_1)}$ is given by the trace of the product: $\langle A, C\rangle_{(\mathcal{B}_\infty,\mathcal{B}_1)} = \operatorname{tr}(AC)$, cf. e. g. [11, Ch. 6] for details.

Assumption 5.1. Let $V_0 \in L^2_{\mathbb{R}}$ from now on be a fixed potential, and let once and for all $\rho \in \mathbb{R}$ be a number such that 1 is a lower form bound of the operator $H_0 + V_0 + V + \rho$ for H_0 from Definition 2.3, and all $V \in L^2_{\mathbb{R}}$ with $\|V\|_{L^2} \leq 1$. Corollary 4.10 ensures the existence of such a ρ.

Definition 5.2. With respect to H_0 from Definition 2.3, and V_0 and ρ from Assumption 5.1 we introduce $H \stackrel{\text{def}}{=} H_0 + V_0 + \rho$. Moreover, $\mathfrak{M} : L^2 \to \mathcal{B}_\infty$ is the linear, continuous mapping $W \mapsto WH^{-1}$, cf. (4.9).

Henceforth we make Assumption 3.4. Then Lemma 4.12 applies, cf. Remark 4.14; thus, the operator $Hf(H_0 + V_0 + V)$ belongs to $\mathcal{B}_1$ for every $V \in L^2_{\mathbb{R}}$. Due to Corollary 4.13 one has for all $W \in L^2$

$$\begin{aligned}\int_\Omega W\mathcal{N}(V_0+V)\,dx &= \operatorname{tr}\big(Wf(H_0+V_0+V)\big)\\ &= \operatorname{tr}\big(WH^{-1}Hf(H_0+V_0+V)\big) = \langle\mathfrak{M}(W), Hf(H_0+V_0+V)\rangle_{(\mathcal{B}_\infty,\mathcal{B}_1)}.\end{aligned}$$

Hence, one can represent the particle density operator in terms of the linear, continuous mapping $\mathfrak{M}^* : \mathcal{B}_1 \to L^2$,

$$\mathcal{N}(V_0+V) = \mathfrak{M}^*(Hf(H_0+V_0+V)) \quad \text{for all } V \in L^2_{\mathbb{R}}. \tag{5.1}$$

Lemma 5.3. *Let $\mathfrak{M}$ and $H = H_0 + V_0 + \rho$ be according to Definition 5.2 and A be a selfajoint operator on L^2 such that $HA \in \mathcal{B}_1$. Then $\mathfrak{M}^*(HA) \in L^2_{\mathbb{R}}$.*

Proof. Given (5.1) it only remains to show that $\mathfrak{M}^*(HA)$ is real valued, or equivalently, that for any $W \in L^\infty_{\mathbb{R}}$ the scalar product $\int_\Omega W\mathfrak{M}^*(HA)\,dx$ has a real value. Indeed, one has

$$\begin{aligned}\int_\Omega W\mathfrak{M}^*(HA)\,dx = \langle\mathfrak{M}(W), HA\rangle_{(\mathcal{B}_\infty,\mathcal{B}_1)} &= \operatorname{tr}\big(WH^{-1}HA\big)\\ &= \operatorname{tr}\big(WA\big) \quad \text{even for all } W \in L^2_{\mathbb{R}}.\end{aligned} \tag{5.2}$$

Thus, splitting $W \in L^\infty_{\mathbb{R}}$ into its positive and negative part, $W = W_+ - W_-$, we may write

$$\operatorname{tr}\big(WA\big) = \operatorname{tr}\big(W_+^{1/2}A\,W_+^{1/2}\big) - \operatorname{tr}\big(W_-^{1/2}A\,W_-^{1/2}\big).$$

Both addends on the right hand side are real, because the operators $W_+^{1/2}A\,W_+^{1/2}$ and $W_-^{1/2}A\,W_-^{1/2}$ are selfadjoint. □

Remark 5.4. The idea of the proof of Theorem 3.7 is to demonstrate the analyticity of the mapping $L^2_{\mathbb{R}} \ni V \mapsto Hf(H_0 + V_0 + V) \in \mathcal{B}_1$ under the Assumption 3.4 by representing

$$Hf(H_0 + V_0 + V) - Hf(H_0 + V_0) \tag{5.3}$$

locally as a series $\sum_{j=1}^{\infty} HT_j(V)$ of j-power mappings, cf. Definition 2.5, such that

- for every $j \in \mathbb{N}$ and $V \in L^2_{\mathbb{R}}$ the operator $T_j(V)$ is nuclear and selfadjoint,
- and $H \sum_{j=1}^{k} T_j(V)$ converges for $k \to \infty$ in $\mathcal{B}_1$ to (5.3).

Then the linear, continuous mappping $\mathfrak{M}^* : \mathcal{B}_1 \to L^2$ carries over this representation in j-power mappings to the mapping

$$L^2_{\mathbb{R}} \ni V \mapsto \mathcal{N}(V_0 + V) - \mathcal{N}(V_0) \in L^2_{\mathbb{R}},$$

ensuring the analyticity of $\mathcal{N}$, cf. Definition 2.5.

Remark 5.5. The analyticity of the mapping

$$L^2_{\mathbb{R}} \ni V \mapsto Hf(H_0 + V_0 + V) \in \mathcal{B}_1$$

is equivalent to the analyticity of the mapping

$$L^2_{\mathbb{R}} \ni V \mapsto f(H_0 + V_0 + V) \in X,$$

where X is the "weighted" Schatten class $\{A \in \mathcal{B} : HA \in \mathcal{B}_1\}$ equipped with the norm $\|A\|_X \stackrel{\text{def}}{=} \|HA\|_{\mathcal{B}_1}$.

In the sequel we show the analyticity of the mapping

$$L^2_{\mathbb{R}} \ni V \mapsto Hf(H_0 + V_0 + V) \in \mathcal{B}_1$$

under the Assumption 3.4. First, we introduce the shifted distribution function $g : \mathbb{C} \to \mathbb{C}$ by

$$g(\lambda) \stackrel{\text{def}}{=} f(\lambda - \rho), \quad \lambda \in \mathbb{C} \tag{5.4}$$

with respect to ρ from Assumption 5.1. Obviously,

$$f(H_0 + V_0 + V) = f(H + V - \rho) = g(H + V).$$

Moreover, with f also g complies with Assumption 3.4, and the function g inherits all properties asserted in Remark 3.5 from the function f. So, let $\alpha > 0$ be a number such that the function g is holomorphic on the set $\mathcal{P}_\alpha - 1$, cf. Definition 3.3, and $\sup_{\lambda \in \mathcal{P}_\alpha - 1} |\lambda^9 g(\lambda)| < \infty$. Then $\int_\Upsilon |\lambda|^7 |g(\lambda)|\, d|\lambda| < \infty$, where Υ is the contour corresponding to $\mathcal{P}_\alpha$ in the sense of Definition 3.3. Note that Υ encloses the spectrum of $H+V$ for all $V \in L^2_{\mathbb{R}}$ with $\|V\|_{L^2} \le 1$, cf. Assumption 5.1. According to the Dunford calculus, cf. e. g. [13, Ch. VII.9], for these V holds

$$g(H+V) = -\frac{1}{2\pi i}\int_\Upsilon g(\lambda)(H+V-\lambda)^{-1}\,d\lambda. \tag{5.5}$$

Applying iteratively the resolvent equation

$$(H+V-\lambda)^{-1} = (H-\lambda)^{-1} - (H-\lambda)^{-1}V(H+V-\lambda)^{-1},$$

we get

$$\begin{aligned}(H+V-\lambda)^{-1} = (H-\lambda)^{-1} + (H-\lambda)^{-1}\sum_{j=1}^{7}(-1)^j\big(V(H-\lambda)^{-1}\big)^j \\ + (H-\lambda)^{-1}\big(V(H-\lambda)^{-1}\big)^7V(H+V-\lambda)^{-1}.\end{aligned} \tag{5.6}$$

The first term of (5.6) corresponds to the term $\mathcal{N}(V_0)$ in the j-power expansion of $\mathcal{N}(V_0+V)$. The operator

$$-\frac{1}{2\pi i}\int_\Upsilon g(\lambda)(H-\lambda)^{-1}\,d\lambda = g(H) = f(H_0+V_0)$$

is bounded and self-adjoint. Moreover, the operator $Hf(H_0+V_0)$ is nuclear, cf. Lemma 4.12.

Lemma 5.6. *For $j \in \mathbb{N}$ and $V \in L^2_{\mathbb{R}}$ we define the j-linear mapping*

$$T_j(V) \stackrel{\text{def}}{=} \frac{(-1)^{j+1}}{2\pi i}\int_\Upsilon g(\lambda)(H-\lambda)^{-1}\big(V(H-\lambda)^{-1}\big)^j\,d\lambda. \tag{5.7}$$

1. *For every $V \in L^2_{\mathbb{R}}$, the operator $HT_j(V)$ is bounded, and*

$$HT_j(V) = \frac{(-1)^{j+1}}{2\pi i}\int_\Upsilon g(\lambda)H(H-\lambda)^{-1}\big(V(H-\lambda)^{-1}\big)^j\,d\lambda. \tag{5.8}$$

   Moreover, every operator $T_j(V)$ is bounded.

2. *For every $V \in L^2_{\mathbb{R}}$, the operator $T_j(V)$ is selfadjoint.*

3. *If $j \in \{1,\dots,7\}$, then the mapping $L^2_{\mathbb{R}} \ni V \mapsto HT_j(V)$ maps $L^2_{\mathbb{R}}$ boundedly into $\mathcal{B}_1$.*

Proof. 1) Observing that $\mathcal{D}$ can be equivalently normed by $\|H\cdot\|_{L^2}$, cf. Definition 2.3, Corollary 4.10, and Corollary 4.11, one estimates

$$\begin{aligned}
&\int_\Upsilon |g(\lambda)| \big\|(H-\lambda)^{-1}\big(V(H-\lambda)^{-1}\big)^j\big\|_{\mathcal{B}(L^2;\mathcal{D})}\, d|\lambda| \\
&\le c\int_\Upsilon |g(\lambda)| \big\|H(H-\lambda)^{-1}\big(V(H-\lambda)^{-1}\big)^j\big\|_{\mathcal{B}}\, d|\lambda| \\
&\le c\int_\Upsilon |g(\lambda)|\, d|\lambda| \, \big(\|V\|_{L^2}\|H^{-1}\|_{\mathcal{B}(L^2;L^\infty)}\big)^j \sup_{\lambda\in\Upsilon}\|H(H-\lambda)^{-1}\|_{\mathcal{B}}^{j+1}
\end{aligned}$$

where the right hand side is finite, thanks to Theorem 4.3, Corollary 4.11 and Lemma 4.1. Thus, integration and the application of H may be interchanged, cf. [41, Ch. IV.4 Thm. 45].

2) One easily verifies for $\lambda\in\Upsilon$ the identity

$$\Big((H-\lambda)^{-1}\big(V(H-\lambda)^{-1}\big)^j\Big)^* = (H-\bar\lambda)^{-1}\big(V(H-\bar\lambda)^{-1}\big)^j. \tag{5.9}$$

Hence, observing Remark 3.6, one gets from (5.7)

$$\begin{aligned}
\big(T_j(V)\big)^* &= \Big(\frac{(-1)^{j+1}}{2\pi i}\int_\Upsilon g(\lambda)(H-\lambda)^{-1}\big(V(H-\lambda)^{-1}\big)^j \frac{d\lambda}{d|\lambda|}\, d|\lambda|\Big)^* \\
&= -\frac{(-1)^{j+1}}{2\pi i}\int_\Upsilon g(\bar\lambda)(H-\bar\lambda)^{-1}\big(V(H-\bar\lambda)^{-1}\big)^j \overline{\frac{d\lambda}{d|\lambda|}}\, d|\lambda|.
\end{aligned}$$

Now the variable transformation $\lambda\mapsto\bar\lambda$ shows that the right hand side is equal to $T_j(V)$.

3) We demonstrate the assertion exemplarily for $HT_2(V)$: Making use of the resolvent equation

$$(H-\lambda)^{-1} = H^{-1} + \lambda H^{-1}(H-\lambda)^{-1} \tag{5.10}$$

we obtain

$$\begin{aligned}
HT_2(V) &= \frac{-H}{2\pi i}\int_\Upsilon g(\lambda)(H-\lambda)^{-1}V(H-\lambda)^{-1}V(H-\lambda)^{-1}\, d\lambda \\
&= \frac{-H}{2\pi i}\int_\Upsilon g(\lambda)(H-\lambda)^{-1}\Big[VH^{-1}VH^{-1} \\
&\qquad + \lambda VH^{-1}(H-\lambda)^{-1}VH^{-1} + \lambda VH^{-1}VH^{-1}(H-\lambda)^{-1} \\
&\qquad + \lambda^2 VH^{-1}(H-\lambda)^{-1}VH^{-1}(H-\lambda)^{-1}\Big]\, d\lambda.
\end{aligned}$$

Now we make use again of the resolvent equation (5.10) in those summands where

$(H-\lambda)^{-1}$ appears exactly once as a factor. Thus,

$$\begin{aligned} HT_2(V) = \frac{-H}{2\pi i}\int_\Upsilon g(\lambda)(H-\lambda)^{-1}\Big[(VH^{-1})^2 + \lambda V(H^{-2}VH^{-1} + H^{-1}VH^{-2}) \\ + \lambda^2 VH^{-2}(H-\lambda)^{-1}VH^{-1} + \lambda^2 VH^{-1}VH^{-2}(H-\lambda)^{-1} \\ + \lambda^2 VH^{-1}(H-\lambda)^{-1}VH^{-1}(H-\lambda)^{-1}\Big]\, d\lambda. \end{aligned}$$

We discuss the summands separately. For the first term we get

$$-\frac{1}{2\pi i}H\int_\Upsilon g(\lambda)(H-\lambda)^{-1}(VH^{-1})^2\, d\lambda = Hg(H)(VH^{-1})^2$$

which belongs to $\mathcal{B}_1$ and admits the estimate

$$\|Hg(H)(VH^{-1})^2\|_{\mathcal{B}_1} \le \|Hg(H)\|_{\mathcal{B}_1}\|V\|_{L^2}^2\|H^{-1}\|^2_{\mathcal{B}(L^2;L^\infty)} \le c\|V\|^2_{L^2}$$

according to Theorem 4.3, Lemma 4.12 and Corollary 4.11. If $\tilde g$ denotes the function $\lambda \mapsto \lambda g(\lambda)$, then

$$\begin{aligned} -\frac{1}{2\pi i}H\int_\Upsilon \lambda g(\lambda)(H-\lambda)^{-1}VH^{-2}VH^{-1}\, d\lambda = H\tilde g(H)VH^{-2}VH^{-1}, \\ -\frac{1}{2\pi i}H\int_\Upsilon \lambda g(\lambda)(H-\lambda)^{-1}VH^{-1}VH^{-2}\, d\lambda = H\tilde g(H)VH^{-1}VH^{-2}, \end{aligned}$$

and one can estimate

$$\begin{aligned} &\|H\tilde g(H)VH^{-2}VH^{-1}\|_{\mathcal{B}_1} + \|H\tilde g(H)VH^{-1}VH^{-2}\|_{\mathcal{B}_1} \\ &\le 2\|H\tilde g(H)\|_{\mathcal{B}_2}\|V\|^2_{L^2}\|H^{-1}\|^2_{\mathcal{B}(L^2;L^\infty)}\|H^{-1}\|_{\mathcal{B}_2} \\ &\le 2\|V\|^2_{L^2}\|H^{-1}\|^2_{\mathcal{B}(L^2;L^\infty)}\|H^{-1}\|^2_{\mathcal{B}_2}\sup_{s\in\operatorname{spec}(H)}|s^3 g(s)| < \infty. \end{aligned}$$

In order to estimate the first of the terms with λ^2 we note that the integral

$$\begin{aligned} &\int_\Upsilon |\lambda^2 g(\lambda)|\|(H-\lambda)^{-1}VH^{-2}(H-\lambda)^{-1}VH^{-1}\|_{\mathcal{B}(L^2;\mathcal{D})}\, d|\lambda| \\ &\le c\int_\Upsilon |\lambda^2 g(\lambda)|\|H(H-\lambda)^{-1}VH^{-2}(H-\lambda)^{-1}VH^{-1}\|_{\mathcal{B}}\, d|\lambda| \\ &\le c\sup_{\lambda\in\Upsilon}\|H(H-\lambda)^{-1}\|^2\|V\|^2_{L^2}\|H^{-2}\|_{\mathcal{B}}\|H^{-1}\|^2_{\mathcal{B}(L^2;L^\infty))}\int_\Upsilon|\lambda^2 g(\lambda)|\, d|\lambda| \end{aligned}$$

is finite. Hence, one has

$$\begin{aligned} -\frac{1}{2\pi i}H\int_\Upsilon \lambda^2 g(\lambda)(H-\lambda)^{-1}VH^{-2}(H-\lambda)^{-1}VH^{-1}\, d\lambda \\ = -\frac{1}{2\pi i}\int_\Upsilon \lambda^2 g(\lambda)H(H-\lambda)^{-1}VH^{-2}(H-\lambda)^{-1}VH^{-1}\, d\lambda \in \mathcal{B}. \end{aligned}$$

Actually, this integral is a nuclear operator, and can be estimated as follows:

$$\begin{aligned}
&\frac{1}{2\pi}\Big\| \int_\Upsilon \lambda^2 g(\lambda) H(H-\lambda)^{-1} V H^{-2} (H-\lambda)^{-1} V H^{-1}\, d\lambda \Big\|_{\mathcal{B}_1} \\
&\le c \int_\Upsilon |\lambda^2 g(\lambda)| \|H(H-\lambda)^{-1} V H^{-1} H^{-2} H (H-\lambda)^{-1} V H^{-1}\|_{\mathcal{B}_1}\, d|\lambda| \\
&\le c \sup_{\lambda\in\Upsilon} \|H(H-\lambda)^{-1}\|_{\mathcal{B}}^2 \|V\|_{L^2}^2 \|H^{-1}\|_{\mathcal{B}(L^2;L^\infty)}^2 \|H^{-1}\|_{B_2}^2 \int_\Upsilon |\lambda^2 g(\lambda)|\, d|\lambda|.
\end{aligned}$$

This is finite, due to Lemma 4.1, Corollary 4.11, Theorem 4.5, and Assumption 3.4. The terms

$$-\frac{1}{2\pi i} H \int_\Upsilon \lambda^2 g(\lambda) (H-\lambda)^{-1} V H^{-1} V H^{-2} (H-\lambda)^{-1}\, d\lambda,$$
$$-\frac{1}{2\pi i} H \int_\Upsilon \lambda^2 g(\lambda) (H-\lambda)^{-1} V H^{-1} (H-\lambda)^{-1} V H^{-1} (H-\lambda)^{-1}\, d\lambda$$

can be treated analogously. □

Remark 5.7. We have demonstrated the third assertion of Lemma 4.1 exemplarily for $HT_2(V)$, thereby using that $\int_\Upsilon |\lambda^2 g(\lambda)|\, d|\lambda|$ is finite. Analogously, one uses that the integral $\int_\Upsilon |\lambda^7 g(\lambda)|\, d|\lambda|$ is finite to prove the assertion for $HT_7(V)$. That is why we asked for $|\lambda|$ to the power of 9 in the supremum condition of Assumption 3.4, cf. Remark 3.5.

Lemma 5.6 shows that the first 7 terms of the expansion of the mapping $V \mapsto Hf(H_0 + V_0 + V) - Hf(H_0 + V_0)$ are j-power mappings. To finalise the proof of Theorem 3.7 it remains to show — according to Definition 2.5 — that the term, cf. (5.5) and (5.6),

$$-\frac{H}{2\pi i} \int_\Upsilon g(\lambda)(H-\lambda)^{-1} \big(V(H-\lambda)^{-1}\big)^7 V (H+V-\lambda)^{-1}\, d\lambda \tag{5.11}$$

may be represented as a series of j-power mappings, uniformly converging in some ball of $L^2_{\mathbb{R}}$. Let us begin with the estimate

$$\begin{aligned}
&\sup_{\lambda\in\Upsilon} \big\| H(H-\lambda)^{-1} \big(V(H-\lambda)^{-1}\big)^7 \big\|_{\mathcal{B}} \\
&\le \sup_{\lambda\in\Upsilon} \big\| H(H-\lambda)^{-1} \big(V(H-\lambda)^{-1}\big)^7 \big\|_{\mathcal{B}_1} \\
&\le \sup_{\lambda\in\Upsilon} \|H(H-\lambda)^{-1}\|_{\mathcal{B}}^8 \|VH^{-1}\|_{\mathcal{B}_7}^7 \\
&\le \tfrac{1}{\operatorname{dist}(1,\Upsilon)^8} \Big(\|V\|_{L^2} \|(H_0+1)^{-\frac{10}{13}}\|_{\mathcal{B}(L^2;L^\infty)} \|(H_0+1)^{-\frac{3}{13}}\|_{\mathcal{B}_7} \|(H_0+1)H^{-1}\|_{\mathcal{B}} \Big)^7 \\
&< \infty,
\end{aligned} \tag{5.12}$$

cf. Lemma 4.1, Corollary 4.8, and Corollary 4.11. This leads to the estimate

$$\begin{aligned}
&\sup_{\lambda\in\Upsilon} \big\|H(H-\lambda)^{-1}\big(V(H-\lambda)^{-1}\big)^7 V(H+V-\lambda)^{-1}\big\|_{\mathcal{B}} \\
&\le \sup_{\lambda\in\Upsilon} \big\|H(H-\lambda)^{-1}\big(V(H-\lambda)^{-1}\big)^7 V(H+V-\lambda)^{-1}\big\|_{\mathcal{B}_1} \\
&\le \sup_{\lambda\in\Upsilon} \big\|H(H-\lambda)^{-1}\big(V(H-\lambda)^{-1}\big)^7\big\|_{\mathcal{B}_1} \sup_{\lambda\in\Upsilon} \|V(H+V-\lambda)^{-1}\|_{\mathcal{B}} \\
&\le c\,\|V\|_{L^2}^7 \|V(H+V)^{-1}\|_{\mathcal{B}} < \infty,
\end{aligned}$$

cf. Corollary 4.11. From this we draw two conclusions: First, the integral

$$\int_\Upsilon |g(\lambda)|\, \|(H-\lambda)^{-1}\big(V(H-\lambda)^{-1}\big)^7 V(H+V-\lambda)^{-1}\|_{\mathcal{B}(L^2;\mathcal{D})}\, d|\lambda|$$

converges. Thus, (5.11) is identical with

$$-\frac{1}{2\pi i}\int_\Upsilon g(\lambda) H(H-\lambda)^{-1}\big(V(H-\lambda)^{-1}\big)^7 V(H+V-\lambda)^{-1}\, d\lambda. \tag{5.13}$$

Second, the integral

$$\int_\Upsilon |g(\lambda)|\, \big\|H(H-\lambda)^{-1}\big(V(H-\lambda)^{-1}\big)^7 V(H+V-\lambda)^{-1}\big\|_{\mathcal{B}_1}\, d|\lambda|$$

also converges. Hence, the mapping, which assigns to $V \in L^2_{\mathbb{R}}$ the expression (5.11), in fact takes its values in $\mathcal{B}_1$.

Now we regard the — for the time being formal — series expansion

$$\begin{aligned}
(H+V-\lambda)^{-1} &= \big((1+V(H-\lambda)^{-1})(H-\lambda)\big)^{-1} \\
&= (H-\lambda)^{-1}\big(1+V(H-\lambda)^{-1}\big)^{-1} = (H-\lambda)^{-1}\sum_{j=0}^{\infty}(-1)^j\big(V(H-\lambda)^{-1}\big)^j,
\end{aligned}$$

and make use of it in (5.13), respectively. This gives for (5.11) the expression

$$-\frac{1}{2\pi i}\int_\Upsilon g(\lambda) H(H-\lambda)^{-1}\big(V(H-\lambda)^{-1}\big)^7 V(H-\lambda)^{-1}\sum_{j=0}^{\infty}(-1)^j\big(V(H-\lambda)\big)^j\, d\lambda. \tag{5.14}$$

According to Lemma 4.1, Theorem 4.3, and Corollary 4.11 there is the inequality

$$\begin{aligned}
\|V(H-\lambda)^{-1}\|_{\mathcal{B}} &\le \|V\|_{L^2}\|H^{-1}\|_{\mathcal{B}(L^2;L^\infty)} \sup_{\lambda\in\Upsilon}\|H(H-\lambda)^{-1}\|_{\mathcal{B}} \\
&\le \tfrac{1}{\mathrm{dist}(1,\Upsilon)}\|V\|_{L^2}\|H^{-1}\|_{\mathcal{B}(L^2;L^\infty)}.
\end{aligned} \tag{5.15}$$

Hence, the series $\sum_{j=0}^{\infty}(-1)^j \big(V(H-\lambda)\big)^j$ absolutely converges in $\mathcal{B}$ if

$$\|V\|_{L^2} < \frac{\operatorname{dist}(1,\Upsilon)}{\|H^{-1}\|_{\mathcal{B}(L^2;L^\infty)}}. \tag{5.16}$$

Consequently, (5.14) holds strictly for those $V \in L^2_{\mathbb{R}}$ agreeing with (5.16).

We investigate now for all $j > 7$ the mappings HT_j, where T_j is given by (5.7). Due to the first assertion of Lemma 5.6, (5.12), and (5.15), HT_j admits the following estimate:

$$\begin{aligned}
&\|HT_j(V)\|_{\mathcal{B}_1}\\
&\le \int_\Upsilon |g(\lambda)| \big\|H(H-\lambda)^{-1}\big(V(H-\lambda)^{-1}\big)^7\big(V(H-\lambda)^{-1}\big)^{j-7}\big\|_{\mathcal{B}_1}\, d|\lambda|\\
&\le \sup_{\lambda\in\Upsilon} \big\|H(H-\lambda)^{-1}\big(V(H-\lambda)^{-1}\big)^7\|_{\mathcal{B}_1} \times\\
&\qquad \times \sup_{\lambda\in\Upsilon} \big\|\big(V(H-\lambda)^{-1}\big)^{j-7}\|_{\mathcal{B}} \int_\Upsilon |g(\lambda)|\, d|\lambda|\\
&\le c\, \|V\|^7_{L^2} \Big(\|V\|_{L^2} \tfrac{\|H^{-1}\|_{\mathcal{B}(L^2;L^\infty)}}{\operatorname{dist}(1,\Upsilon)}\Big)^{j-7}.
\end{aligned}$$

Thus, HT_j is a j-power mapping from $L^2_{\mathbb{R}}$ into $\mathcal{B}_1$ for every $j > 7$. Moreover, for $V \in L^2_{\mathbb{R}}$ satisfying (5.16), the series

$$\sum_{j=8}^{\infty} \int_\Upsilon |g(\lambda)| \big\|H(H-\lambda)^{-1}\big(V(H-\lambda)^{-1}\big)^7\big(V(H-\lambda)^{-1}\big)^{j-7}\|_{\mathcal{B}_1}\, d|\lambda|$$

converges. Thus, for $V \in L^2_{\mathbb{R}}$ satisfying (5.16) one may interchange summation and integration in (5.14) (cf. e. g. [41, Ch. IV.4 Thm. 37]). Therefore, (5.11) is an absolutely converging series

$$-\frac{H}{2\pi i}\int_\Upsilon g(\lambda)(H-\lambda)^{-1}\big(V(H-\lambda)^{-1}\big)^7 V(H+V-\lambda)^{-1}\, d\lambda = \sum_{j=8}^{\infty} HT_j(V)$$

in $\mathcal{B}_1$ for all $V \in L^2_{\mathbb{R}}$ satisfying (5.16). As a result $\sum_{j=1}^{\infty} HT_j(V)$ converges absolutely and uniformly in $\mathcal{B}_1$ for all $V \in L^2_{\mathbb{R}}$ with $\|V\|_{L^2} < c < \operatorname{dist}(1,\Upsilon)/\|H^{-1}\|_{\mathcal{B}(L^2;L^\infty)}$. If, additionally, $\|V\|_{L^2} \le 1$, then

$$Hf(H_0+V_0+V) = Hf(H_0+V_0) + \sum_{j=1}^{\infty} HT_j(V)$$

according to the Dunford calculus, cf. (5.5). Now the conclusion of Remark 5.4 finishes the proof of Theorem 3.7.

6 Concluding remarks

Theorem 4.3 restricts the dimension of the spatial domain Ω to 1, 2, and 3, cf. Remark 4.4. On the other hand these are just the dimensions we are involved with in the underlying real space representation of quantum mechanics.

The proofs in this paper have been done in such a way that they work simultaneously for the space dimensions $d = 1, 2, 3$, and the decay properties of the thermodynamic equilibrium distribution function f we impose in Assumption 3.4 are accordingly. However, the spatially one- and two-dimensional case could be treated more easily separately assuming less. This is due to the fact that for $d = 1, 2$ one has better summability of the resolvent of an elliptic operator, and more regularity for the solution of an elliptic PDE.

Remark 6.1. The first term of the j-power expansion of the mapping

$$V \mapsto Hf(H_0 + V_0 + V) - Hf(H_0 + V_0)$$

corresponds to the Fréchet derivative of the operator function

$$V \mapsto f(H_0 + V_0 + V).$$

Hence, the Fréchet derivative $\partial\mathcal{N}$ of the particle density operator $\mathcal{N}$, cf. Definition 3.1, is given by

$$\partial\mathcal{N}(V_0)[V] = \mathfrak{M}^*\big(HT_1(V)\big) \quad \text{for all } V_0,\, V \in L^2_{\mathbb{R}}, \tag{6.1}$$

where H is according to Definition 5.2, cf. Remark 5.4 and Definition 2.5. Thus, we can conclude from Lemma 5.6 and (5.2)

$$\begin{aligned} \int_\Omega W\partial\mathcal{N}(V_0)[V]\,dx = \int_\Omega W\mathfrak{M}^*\big(HT_1(V)\big)\,dx = \operatorname{tr}\big(WT_1(V)\big) \\ = \frac{1}{2\pi i}\int_\Upsilon g(\lambda)\operatorname{tr}\big(W(H-\lambda)^{-1}V(H-\lambda)^{-1}\big)\,d\lambda \end{aligned} \tag{6.2}$$

for all V_0, $V \in L^2_{\mathbb{R}}$ and all $W \in L^2_{\mathbb{R}}$, where $H = H_0 + V_0 + \rho$, and ρ is a number such that 1 is a lower form bound of $H_0 + V_0 + V + \rho$. The function g is according to (5.4). Moreover, Υ is a contour in the sense of Definition 3.3 which includes all eigenvalues of $H_0 + V_0 + V + \rho$. If $\{\lambda_k\}$ is the sequence of eigenvalues for $H_0 + V_0$ (counting multiplicity) and $\{\psi_k\}$ is the corresponding sequence of (normalized) eigenvectors, then

$$\begin{aligned} &\operatorname{tr}\big(W(H-\lambda)^{-1}V(H-\lambda)^{-1}\big) \\ &\qquad = \sum_{k,\ell=1}^{\infty} \frac{1}{(\lambda_k+\rho-\lambda)(\lambda_\ell+\rho-\lambda)}\langle W\psi_k,\psi_\ell\rangle_{L^2}\langle V\psi_\ell,\psi_k\rangle_{L^2}, \end{aligned}$$

cf. e. g. [36], [24, §6.5]. Thus, one obtains from (6.2)

$$\int_\Omega W \partial\mathcal{N}(V_0)[V]\,dx = \sum_{\substack{k,\ell=1\\ \lambda_k=\lambda_\ell}}^{\infty} f'(\lambda_k)\langle W\psi_k,\psi_\ell\rangle_{L^2}\langle V\psi_\ell,\psi_k\rangle_{L^2} + \sum_{\substack{k,\ell=1\\ \lambda_k\neq\lambda_\ell}}^{\infty} \tfrac{f(\lambda_k)-f(\lambda_\ell)}{\lambda_k-\lambda_\ell}\langle W\psi_k,\psi_\ell\rangle_{L^2}\langle V\psi_\ell,\psi_k\rangle_{L^2}. \quad (6.3)$$

Remark 6.2. If the distribution function f, in addition to Assumption 3.4, is strictly monotone, then (6.3) implies

$$\int_\Omega V \partial\mathcal{N}(V_0)[V]\,dx = \sum_{\substack{k,\ell=1\\ \lambda_k=\lambda_\ell}}^{\infty} f'(\lambda_k)\left|\langle V\psi_\ell,\psi_k\rangle_{L^2}\right|^2 + \sum_{\substack{k,\ell=1\\ \lambda_k\neq\lambda_\ell}}^{\infty} \tfrac{f(\lambda_k)-f(\lambda_\ell)}{\lambda_k-\lambda_\ell}\left|\langle V\psi_\ell,\psi_k\rangle_{L^2}\right|^2 < 0$$

for all $V \in L^2_{\mathbb{R}}$ which do not vanish identically. Thus, the particle density operator $\mathcal{N}$, cf. Definition 3.1, is injective due to

$$\int_\Omega \big(\mathcal{N}(V_1)-\mathcal{N}(V_2)\big)(V_1-V_2)\,dx = \int_0^1\int_\Omega \big(\partial\mathcal{N}(V_2+t(V_1-V_2))[V_1-V_2]\big)(V_1-V_2)\,dx\,dt < 0,$$

cf. the proof of Lemma 1.1 in [15, Ch. 3].

Remark 6.3. If N is a given amount of particles in the system, then one calls a number $\epsilon = \epsilon(V)$ which satisfies

$$\int_\Omega \sum_{k=1}^{\infty} f(\lambda_k)|\psi_k|^2\,dx = \sum_{k=1}^{\infty} f(\lambda_k-\epsilon) = N,$$

a Fermi level of the system. If the distribution function f is strictly decreasing, then the Fermi level is uniquely determined. It has been proved in [36], [24] that the Fermi level is continuously Fréchet differentiable on compact subsets of $L^2_{\mathbb{R}}$. We conject the analyticity of the Fermi level with respect to the potential in the Schrödinger operator. The adequate instrument for proving this would be the implicit function theorem, which also works in the context of analytic mappings between Banach spaces, see [44, Ch. 22].

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